ABSTRACT

A computational approach to identifying potential antimicrobial drug targets based on the structural capabilities of the microbe's metabolic network, which may be reconstructed from genomic and biochemical information. Starting with a cellular metabolic network (i) a stoichiometric matrix is generated to describe the connectivity of the reaction in the network, where (ii) constraints can be placed on various fluxes to allow for defined inputs and outputs to the network. For the defined network the unique set of extreme pathways can together be used to describe the complete range of metabolic capabilities of the network. From these pathways, sets of reactions whose elimination from the network removes certain production capabilities from the network can be mathematically determined by process of convex analysis.